REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
15-05-2019	Final Report	3-Jun-2018 - 29-May-2019

4. TITLE AND SUBTITLE
Final Report: Computing System for the Simulation of Multiphases Proceses

5a. CONTRACT NUMBER
W911NF-18-1-0228

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
611103

6. AUTHORS

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES
Rensselaer Polytechnic Institute
110 8th Street

Troy, NY 12180 -3522

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSOR/MONITOR'S ACRONYM(S)
ARO

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
72246-MA-RIP.1

12. DISTRIBUTION AVAILIBILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Mark Shephard
UU	UU	UU	UU		19b. TELEPHONE NUMBER 518-276-8044

RPPR Final Report
as of 16-May-2019

Agency Code:

Proposal Number: 72246MARIP **Agreement Number: W911NF-18-1-0228**

INVESTIGATOR(S):

Name: Assad Oberai
Email: aoberai@usc.edu
Phone Number: 2187401882
Principal:

Name: Onkar S. Sahni
Email: sahni@rpi.edu
Phone Number: 5182768560
Principal:

Name: Mark S. Shephard shephard@s
Email: shephm@rpi.edu
Phone Number: 5182768044
Principal: Y

Organization: **Rensselaer Polytechnic Institute**
Address: 110 8th Street, Troy, NY 121803522
Country: USA

DUNS Number: 002430742 EIN: 141340095
Report Date: 29-Aug-2019 Date Received: 15-May-2019
Final Report for Period Beginning 03-Jun-2018 and Ending 29-May-2019
Title: Computing System for the Simulation of Multiphases Proceses
Begin Performance Period: 03-Jun-2018 **End Performance Period:** 29-May-2019
Report Term: 0-Other
Submitted By: Mark Shephard Email: shephm@rpi.edu
Phone: (518) 276-8044
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: **STEM Participants:**

Major Goals: This DURIP project provided funds for computing hardware to upgrade the computing capabilities of Rensselaer's Scientific Computation Research Center (SCOREC). The primary driver for the requested system is our ongoing U.S. Army Research Office grant entitled "Multiscale Methods for the Reliable Simulation of Multiphase Processes", W911NF-14-1-0301, Professors Assad A. Oberai, Mark S. Shephard and Onkar Sahni Principal Investigators. In addition to the core research, SCOREC has partnered with Simmetrix Inc. on a STTR project entitled "Tools for Parallel Adaptive Simulation of Multiphase Ballistic Flows", W911NF-16-C-0117, for which a Sequential Phase II project will be funded. The efforts in these projects are directly related to supporting the U.S. Army's modernization priorities related to long-range precision fires. As part of these efforts we have developed collaborations with Donald E. Carlucci, Senior Research Scientist, U.S. Army ARDEC RDAR-DSM and Robert E. Dillon, Chief Science Advisor, U.S. Army ARDEC, RDAR-WSB and selected scientist working in their organizations.

In addition, we have an ongoing DoD HPCMP PETTT project supporting the advancement and integration of our adaptive meshing technologies with CREATE-AV Helios code (under AMRDEC's Aviation Development Directorate) and Proteus code (of ERDC's Coastal and Hydraulics Lab). Furthermore, we have initiated efforts to address specific simulation needs of future vertical lift platforms working with Rajneesh Singh, Team Lead, Vehicle Integrated Analysis, U.S. ARL-VTD and Russell Gray, Program Manager, Advanced Programs, Sikorsky Innovations. In this area, we have interacted with the U.S. Army and Sikorsky to perform complex simulations.

Accomplishments: Computing System Upgrades Support by DURIP

The funds from the DURIP grant supported the purchase of a parallel computing cluster, two large memory compute systems and six high-end graphics workstations.

RPPR Final Report
as of 16-May-2019

Parallel Compute Cluster: The parallel compute cluster purchased with the DURIP funds consists of 11 Dell R7425 compute nodes, each with two 24-core 2.3 GHz AMD EPYC processors, 128 GB of DDR4 2666MHz RAM, and a direct connection to a 100Gbps Infiniband fabric. Each node has a peak of 2.2 TerraFLOPS, with an aggregate performance about 24.2 TeraFLOPS. The cluster use in the execution of out large-scale parallel simulation such as those outlined below.

Large Memory Systems: Two Dell R7425 compute nodes with 512GB of RAM were purchased to serve the role of large memory systems. They are otherwise identical to the parallel compute hardware and can be used to provide an additional 4.4 Terraflops for exceptionally demanding computations. In addition to providing addition parallel compute power, the large memory systems support situations that arise where access to a large single address spaces is needed. A common example of this are cases where we are provided extremely large serial mesh cases that we must first process into a distributed mesh for execution of our simulations on the cluster. There are also some secondary codes we use (e.g., partitioners) that either require the large memory access to execute or show poor scaling to high core counts.

Workstations: Six high-end graphics workstations that greatly increase our ability to prepare simulations, develop code, and visualize results were also added to the SCOREC system as part of this project. Each workstation has an Intel Core i7 3.6 GHz 4-core processor, 24 GB of DDR4 2400MHz RAM, and either 4GB Nvidia Quadro P1000 (4) or 8GB Nvideo Quadro P4000 (2) graphics card driving a 27” Dell Ultrasharp 2560x1440 resolution monitor. The two systems with the 8GB Nvideo Quadro P4000 GPU are specifically targeted to support our efforts to develop GPU based version of SCOREC codes as we prepare for the coming generations of massively parallel systems which are heterogeneous systems with GPU accelerators.

Summary of Technology Developments and Results

The focus of our U.S. Army Research Office grant is the development of high-fidelity simulation technologies for propellant burn, and interior and exterior ballistics [1][2][3] [9][10][13][14]. Building on our existing stabilized finite element based CFD capabilities, developments carried out have included:

- A discontinuous Galerkin (DG) method that is only applied at the phase-change interface.
- Arbitrary Eulerian Lagrangian (ALE) formulation with large motion.
- Parallel mesh motion algorithm capable of maintaining element quality as objects change shape and position due to burning and/or motion.
- Parallel mesh adaptation applied on selected time steps when either the mesh quality due to objects shape change and/or motion, or when the discretization errors indicate the mesh topology must change.

The capabilities have been implemented in our parallel, stabilized finite element code called PhaseChangePHASTA. This code has been used to solve compressible flow problems on moving meshes for evolving domains (including phase change) and has been integrated with the geometry tracking methods and meshing technologies developed by Simmetrix in the STTR project.

The attached pdf report includes test examples of a projectile moving down a barrel and propellent burn. The report also discusses our planned continued developments.

Training Opportunities: The systems are currently being used by the three graduate students working on the ARO project to continue the methods development and to run test cases. We are also setting up access to the ARDEC collaborators. The two students and postdoc involved with the PETTT project are using the systems to develop and exercise adaptive methods. A number of other SCOREC postdocs and students have access to the system to do core parallel unstructured mesh technology developments used in PhaseChangePHASTA and the associated mesh adaptation tools.

Results Dissemination: PhaseChangePHASTA and our parallel unstructured mesh adaptation tools are available as open source code under a BSD license. Select faculty, postdocs and students are actively engaged in working with Army researchers on supporting their use of these technologies.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: In addition to technical publications, PhaseChangePHASTA and our parallel unstructured mesh adaptation tools are available as open source code under a BSD license. Select faculty, postdocs and students are actively engaged in working with Army researchers on supporting their use of these technologies.

PARTICIPANTS:

Participant Type: PD/PI
Participant: Mark S. Shephard
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Co PD/PI
Participant: Assad A. Oberai
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Co PD/PI
Participant: Onkar Sahni
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Final Report
Computing System for the Simulation of Multiphase Processes
Grant Number W911NF-18-1-0228

Introduction

This DURIP project provided funds for computing hardware to upgrade the computing capabilities of Rensselaer's Scientific Computation Research Center (SCOREC). The primary driver for the requested system is our ongoing U.S. Army Research Office grant entitled "Multiscale Methods for the Reliable Simulation of Multiphase Processes", W911NF-14-1-0301, Professors Assad A. Oberai, Mark S. Shephard and Onkar Sahni Principal Investigators. In addition to the core research, SCOREC has partnered with Simmetrix Inc. on a STTR project entitled "Tools for Parallel Adaptive Simulation of Multiphase Ballistic Flows", W911NF-16-C-0117, for which a Sequential Phase II project will be funded. The efforts in these projects are directly related to supporting the U.S. Army's modernization priorities related to long-range precision fires. As part of these efforts we have developed collaborations with Donald E. Carlucci, Senior Research Scientist, U.S. Army ARDEC RDAR-DSM and Robert E. Dillon, Chief Science Advisor, U.S. Army ARDEC, RDAR-WSB and selected scientist working in their organizations.

In addition, we have an ongoing DoD HPCMP PETTT project supporting the advancement and integration of our adaptive meshing technologies with CREATE-AV Helios code (under AMRDEC's Aviation Development Directorate) and Proteus code (of ERDC's Coastal and Hydraulics Lab). Furthermore, we have initiated efforts to address specific simulation needs of future vertical lift platforms working with Rajneesh Singh, Team Lead, Vehicle Integrated Analysis, U.S. ARL-VTD and Russell Gray, Program Manager, Advanced Programs, Sikorsky Innovations. In this area, we have interacted with the U.S. Army and Sikorsky to perform complex simulations.

Computing System Upgrades Support by DURIP

The funds from the DURIP grant supported the purchase of a parallel computing cluster, two large memory compute systems and six high-end graphics workstations.

Parallel Compute Cluster: The parallel compute cluster purchased with the DURIP funds consists of 11 Dell R7425 compute nodes, each with two 24-core 2.3 GHz AMD EPYC processors, 128 GB of DDR4 2666MHz RAM, and a direct connection to a 100Gbps Infiniband fabric. Each node has a peak of 2.2 TerraFLOPS, with an aggregate performance about 24.2 TeraFLOPS. The cluster use in the execution of out large-scale parallel simulation such as those outlined below.

Large Memory Systems: Two Dell R7425 compute nodes with 512GB of RAM were purchased to serve the role of large memory systems. They are otherwise identical to the parallel compute hardware and can be used to provide an additional 4.4 Terraflops for exceptionally demanding computations. In addition to providing addition parallel compute power, the large memory systems support situations that arise where access to a large single address spaces is needed. A common example of this are cases where we are provided extremely large serial mesh cases that we must first process into a distributed mesh for execution of our simulations on the cluster. There are also some secondary codes we use (e.g., partitioners) that either require the large memory access to execute or show poor scaling to high core counts.

Workstations: Six high-end graphics workstations that greatly increase our ability to prepare simulations, develop code, and visualize results were also added to the SCOREC system as part of this project. Each workstation has an Intel Core i7 3.6 GHz 4-core processor, 24 GB of DDR4 2400MHz RAM, and either 4GB Nvidia Quadro P1000 (4) or 8GB Nvideo Quadro P4000 (2) graphics card driving a 27" Dell Ultrasharp 2560x1440 resolution monitor. The two systems with the 8GB Nvideo Quadro P4000 GPU are specifically targeted to support our efforts to develop GPU based version of SCOREC codes as we prepare for the coming generations of massively parallel systems which are heterogeneous systems with GPU accelerators.

Summary of Technology Developments and Results

The focus of our U.S. Army Research Office grant is the development of high-fidelity simulation technologies for propellant burn, and interior and exterior ballistics [1][2][3] [9][10][13][14]. Building on our existing stabilized finite element based CFD capabilities, developments carried out have included:

- A discontinuous Galerkin (DG) method that is only applied at the phase-change interface.
- Arbitrary Eulerian Lagrangian (ALE) formulation with large motion.
- Parallel mesh motion algorithm capable of maintaining element quality as objects change shape and position due to burning and/or motion.
- Parallel mesh adaptation applied on selected time steps when either the mesh quality due to objects shape change and/or motion, or when the discretization errors indicate the mesh topology must change.

The capabilities have been implemented in our parallel, stabilized finite element code called PhaseChangePHASTA. This code has been used to solve compressible flow problems on moving meshes for evolving domains (including phase change) and has been integrated with the geometry tracking methods and meshing technologies developed by Simmetrix in the STTR project.

Figure 1 demonstrates the evolution of the geometric model configuration as a projectile moves down a barrel. Sliding contact is supported by evolving the trimmed definition of the surface on which the body slides (the leading and trailing barrel surfaces around the projectile). The projectile may also slide over holes that model muzzle brakes in the barrel.

Figure 2 shows the evolution of the mesh (including a cross-section) as the projectile in Figure 1 moves down the barrel. The mesh is adapted to the size control attributes as the domain evolves: refinement is retained around the projectile, and coarsening carried out behind the projectile as it moves forward. Figure 3 shows an example demonstrating propellant grains undergoing arbitrary motion and deformation in a distributed parallel simulation with the presence of structured layered elements around the phase interface.

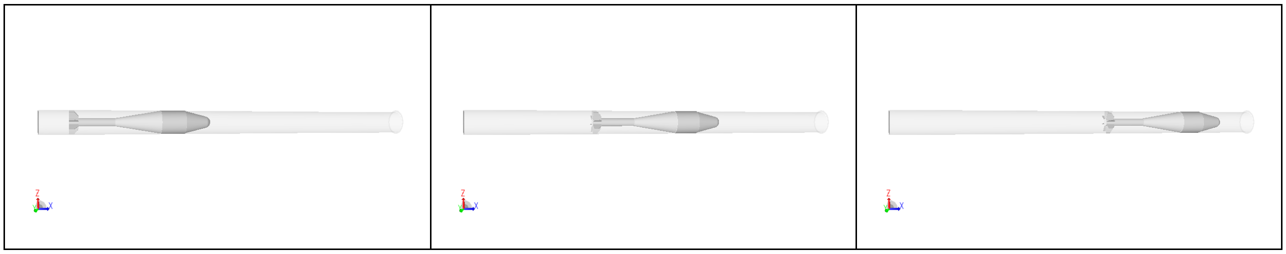

Figure 1: Geometric model evolution as a finned projectile moves down barrel.

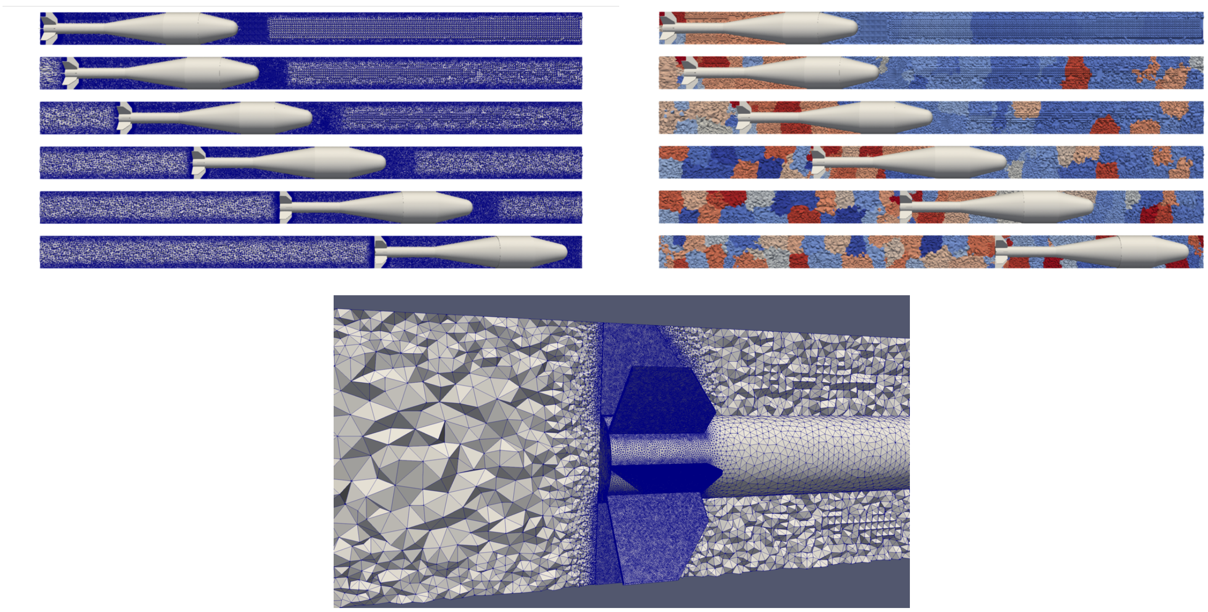

Figure 2: Mesh evolution as a finned projectile moves down barrel: mesh (left top) and partitioning (right top); a zoomed view near the fins at an intermediate instance (bottom).

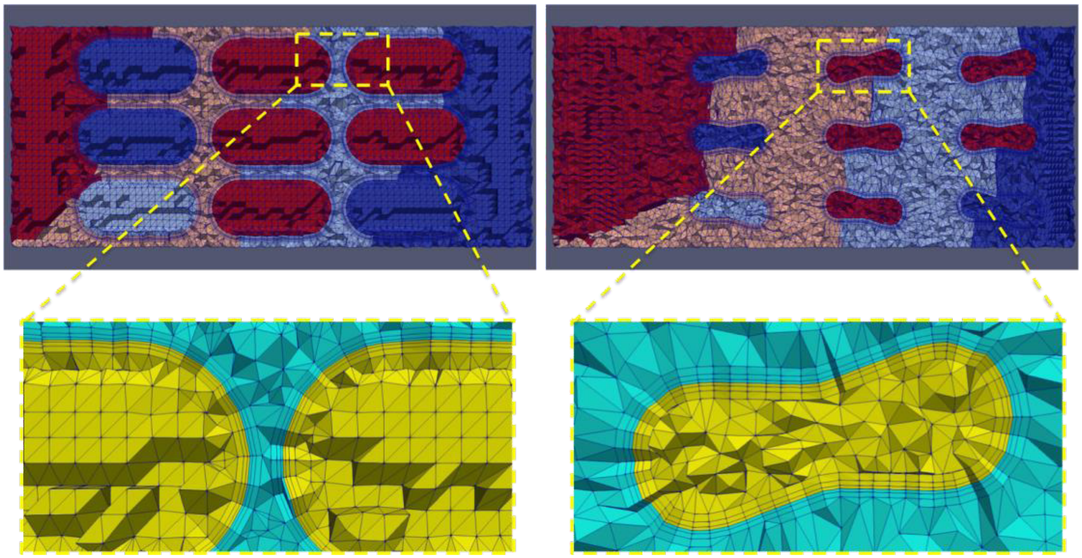

Figure 3: A prescribed mesh motion in parallel for a case with 9 (non-perforated) grains using GeomSim Discrete for deformations (note colors in the top row represent different parts of the partitioned mesh while colors in the bottom row are used to show different phases).

In Figure 4 and Figure 5, we show some of our recent results on grain-burn and moving projectile problems, respectively, based on the PhaseChangePHASTA code together with Simmetrix tools.

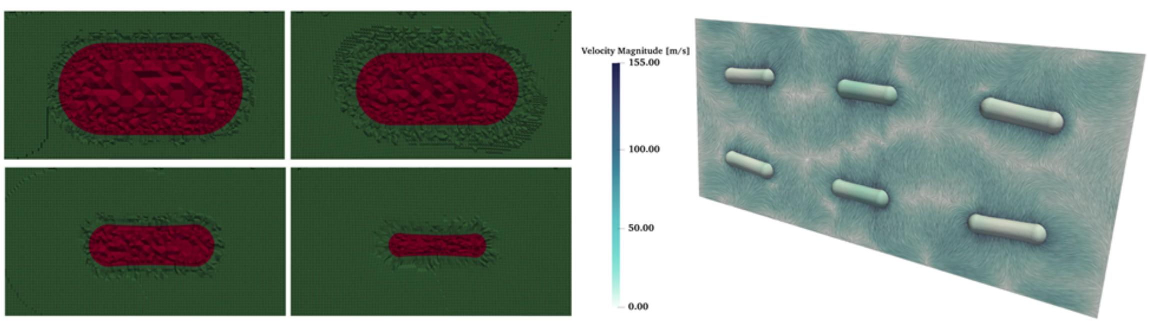

Figure 4: Simulation of physics-driven burn of 6 (non-perforated) grains in a cavity; cross-section view of the mesh for a grain at 4 instances (left) and flow field around 6 grains at the last instance (right).

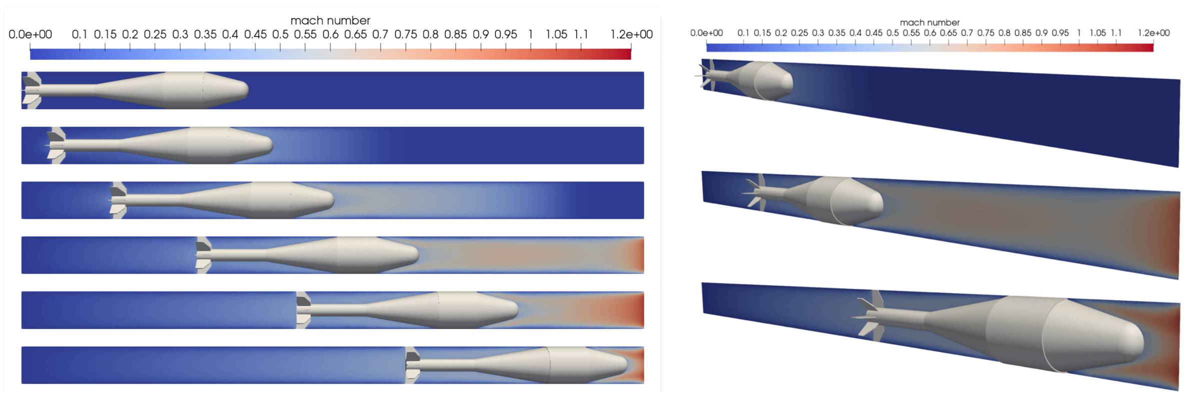

Figure 5: Solution evolution (Mach number) as a finned projectile moves down the barrel (including a 3D view on the right).

In addition to precision fires, we have begun to address specific simulation needs of future vertical lift platforms [4][5][6][7][8][11][12].

Planned Continuing Developments:

Our planned research on the ARO project, for which we are applying for a two year add-on, included efforts in the following areas:

- Extending the current multiphase model to allow us to distinguish between the propellant gas phase, the unburnt air and the products of combustion for a more accurate modeling of the combustion processes.
- A more accurate model of the propellant going from a highly viscous fluid model to a thermoelastic solid undergoing finite deformation.
- A more complete set of adaptive error estimation and adaptive mesh control methods.
- Inclusion of an operator to capture strong shocks that can work in conjunction with specialized mesh adaptation for the accurate resolution of shocks.
- Accounting for model topological changes (such as grains completely burning out, or when the projectile leaves the barrel) within the analysis code and error estimation procedures.

The planned activities on the proposed the Sequential Phase II STTR project include:

- Maintaining consistent geometric fidelity in simulations with evolving geometry and development of reference geometry to be used in adaptive mesh control.
- Generation and adaptation of highly anisotropic meshes for the accurate resolution of key flow physics in thin sections that are orders of magnitude smaller than the geometric entities that enclose/bound the thin sections.
- Parallel construction of non-conforming adaptation and coupling to near-body unstructured meshes of coordinate-aligned octree meshes.
- Improvement of the non-linear solution procedure through the use of better conditioned stabilization operators and more advanced linear algebra technologies.
- Implementation of a base model to account for surface regression of a driving/rotating band as the projectile traverses down the barrel.

A critical part of the above activities will be the demonstration, and subsequent application, of the tools including:

- Prediction of high-speed multiphase flows in long-range precision fires based on high-fidelity simulations of the 3D grain burn process for perforated propellants as well as high-speed flows in narrow gaps and in exterior ballistics in coordination with the U.S. Army ARDEC RDAR-DSM and RDAR-WSB labs.
- Targeted vertical lift problems with complex aerodynamic interactions working with the U.S. Army Research Labs and Sikorsky.

References

[1] R.A. Carson and O. Sahni, "Numerical Investigation of Propellant Leak Methods in Large Caliber Cannons for Blast Overpressure Attenuation", *Shock Waves*, 24(6):625-638, 2014.

[2] R.A. Carson and O. Sahni, “Study of the Relevant Geometric Parameters of the Channel Leak Method for Blast Overpressure Attenuation for a Large Caliber Cannon”, *Computers and Fluids*, 115:211-225, 2015.

[3] R.A. Carson and O. Sahni, “Numerical Investigation of Channel Leak Geometry for Blast Overpressure Attenuation in a Muzzle Loaded Large Caliber Cannon”, Journal of Fluids Engineering, 137(2), 021102 1-12, 2015.

[4] M. Misiorowski, F. Gandhi and A. Oberai, “Computational Analysis and Flow Physics of a Ducted Rotor in Edgewise Flight”, *Proceedings of the 73rd AHS Forum*, Fort Worth, TX, USA, May 2017.

[5] Misiorowski, M., Gandhi, F., and Oberai, A., “A Computational Study on Diffuser Length Variation for a Ducted Rotor in Hover and Edgewise Flight”, *Proceedings of the American Helicopter Society Aeromechanics Specialists Meeting, San Francisco*, CA, USA, Jan. 2018.

[6] Misiorowski, M., Gandhi, F., and Oberai, A., “Computational Analysis of Rotor Interactional Effects for a Quadcopter in Hover and Forward Flight”, *Proceedings of the 74th AHS Forum*, Phoenix, AZ, May 2018.

[7] Misiorowski, M., Gandhi, F., and Oberai, A., “Computational Analysis and Flow Visualization of Ducted Rotors in Edgewise Flight”, *AHS Journal*, 2018, *submitted*.

[8] J. Rane and O. Sahni, “Large Eddy Simulation of Surging Airfoils at High Advance Ratio and Reynolds Number”, *Proceedings of the AIAA Aviation 2018: Aviation and Aeronautics Forum and Exposition*, Atlanta, GA, USA, June 2018.

[9] Sahni, O., Ovcharenko, A., Chitale, K.C., Jansen, K.E. and Shephard, M.S., 2017. Parallel anisotropic mesh adaptation with boundary layers for automated viscous flow simulations. *Engineering with Computers*, *33*(4), pp.767-795.

[10] Smith, C.W., Granzow, B., Diamond, G., Ibanez, D., Sahni, O., Jansen, K.E. and Shephard, M.S., 2018. In-memory integration of existing software components for parallel adaptive unstructured mesh workflows. *Concurrency and Computation: Practice and Experience*, *30*(18), p.e4510.

[11] S. Tendulkar, M.W. Beall, R. Nastasia, O. Sahni, S. Tran and M.S. Shephard. “Advanced meshing and mesh adaptation for complex flow problems”, *Proc. NAFEMS World Congress,* San Diego, CA, 16 pages, 2015.

[12] S.A. Tran, D. Corson and O. Sahni, “Synthetic Jet based Active Flow Control of Dynamic Stall Phenomenon on Wind Turbines Under Yaw Misalignment”, *Proceedings of the AIAA SciTech 2014: Science and Technology Forum and Exposition*, National Harbor, MD, USA, Jan. 2014.

[13] F. Yang, A. Chandra, Y. Zhang, S. Tendulkar, R. Nastasia, A.A. Oberai, Assad Oberai, M.S. Shephard and O. Sahni, “A Parallel Interface-tracking Approach for Moving Boundary Problems”, *Engineering with Computers*, under review.

[14] Y. Zhang, A. Chandra, Fan Yang, Ehsan Shams, Onkar Sahni, M.S. Shephard and A.A. Oberai, “A Locally Discontinuous ALE Finite Element Formulation for Compressible Phase Change Problems”, *Journal of Computational Physics*, under revision.